Rough surface scattering in many-mode conducting channels: gradient versus amplitude scattering

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Abstract

We study the effect of surface scattering on transport properties in many-mode conducting channels (electron waveguides). Assuming a strong roughness of the surface profiles, we show that there are two independent control parameters that determine statistical properties of the scattering. The first parameter is the ratio of the amplitude of the roughness to the transverse width of the waveguide. The second one, which is typically omitted, is determined by the mean value of the derivative of the profile. This parameter may be large, thus leading to specific properties of scattering. Our results may be used in experimental realizations of the surface scattering of electron waves, as well as for other applications (e.g., for optical and microwave waveguides).

Recent numerical studies of quasi-1D disordered systems [1, 2] have revealed principal difference between surface and bulk scattering (see, e.g., discussion and references in [3]). Specifically, it was found that transport properties of quasi-1D waveguides with rough surfaces essentially depend on many characteristic lengths, in contrast to the bulk scattering where one-parametric scaling is determined by the ratio of the localization length to the lengthwise size of samples. This fact is due to a non-isotropic character of surface scattering in the "channel space". In particular, the transmission coefficient smoothly decreases with an increase of the angle of incoming waves, see details in [2, 4]. Below we present an analytical treatment of the electron/wave scattering in waveguides with rough surfaces, paying main attention to the interplay between "amplitude" and "gradient" scattering mechanisms [5, 6].

Our model under consideration is a plane waveguide (or conducting quasi-one-dimensional wire) of average width d, that stretches along the x-axis. The lower boundary of the waveguide is defined as $z = \sigma\xi_1(x)$, while the upper boundary has the profile $z = d+\sigma\xi_2(x)$. Therefore, the width $d(x)$ of the waveguide is $d(x) = d+\sigma[\xi_2(x)-\xi_1(x)]$ with $\langle d(x)\rangle = d$. For random functions $\xi_1(x)$ and $\xi_2(x)$ we assume $\langle \xi_1(x)\rangle = \langle \xi_2(x)\rangle = 0$ and $\langle \xi_1^2(x)\rangle = \langle \xi_2^2(x)\rangle = 1$, so that σ takes the meaning of the root-mean-square roughness height. Here the angular brackets stand for the averaging over x for specific realizations of profiles $\xi_{1,2}(x)$ (or over different realizations of $\xi_{1,2}(x)$). In what follows we consider three cases that reveal generic characteristics of the surface scattering: (A) only the upper profile is rough, $\xi_1(x) = 0$ and $\xi_2(x) = \xi(x)$; (B) two profiles are asymmetrical, $\xi_1(x) = \xi_2(x) = \xi(x)$, in respect to the central line $z = d/2$; (C) two profiles are symmetrical, $-\xi_1(x) = \xi_2(x) = \xi(x)$. Note, however, that our approach is valid for any profiles $\xi_1(x)$ and $\xi_2(x)$.

The method we use is based on the coordinate transformation that makes both boundaries flat, (see for example, [6, 7]),

$$x_{new} = x_{old} = x, \qquad z_{new} = \frac{[z_{old} - \sigma\xi_1(x)]d}{d(x)}. \tag{1}$$

Let us start with the case (A) when one surface is flat and the other has the roughness that is assumed to be defined by the Gaussian random function $\xi(x)$ with the binary correlator $\langle \xi(x)\xi(x')\rangle = \mathcal{W}(x - x')$. The latter is normalized to its maximal value, $\mathcal{W}(0) = 1$, and supposed to decrease on a characteristic scale R_c. Since $\mathcal{W}(x)$ is an even function of x, its Fourier transform $W(k_x) = \int_{-\infty}^{\infty} dx\, \exp(-ik_x x)\, \mathcal{W}(x)$ is even, real and non-negative function

of the lengthwise wave number k_x. The roughness power spectrum $W(k_x)$ has a maximum $W(0) \sim R_c$ at $k_x = 0$, and decreases on the scale R_c^{-1} as $|k_x|$ increases.

In order to solve the scattering problem we employed the method of the Green's function $\mathcal{G}(x, x'; z, z')$ for which the equation has the form,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2\right) \mathcal{G}(x, x'; z, z') = \delta(x - x')\delta(z - z'), \tag{2}$$

with the boundary conditions $\mathcal{G}(x, x'; z = 0, z') = \mathcal{G}(x, x'; z = d(x), z') = 0$. The wave number k is equal to ω/c for a classical scalar wave of frequency ω, and is the Fermi wave number for electrons in the isotropic Fermi-liquid model.

After transformation to new variables the equation for the canonically conjugated Green's function gets the following form (below we use notation z instead of z_{new}),

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2\right) \mathcal{G}(x, x'; z, z') - \left\{\left[1 - \frac{d^2}{d^2(x)}\right]\frac{\partial^2}{\partial z^2} + \frac{\sigma\hat{\mathcal{U}}(x)}{d(x)}\left[\frac{1}{2} + z\frac{\partial}{\partial z}\right]\right.$$
$$\left. -\frac{\sigma^2\xi'^2(x)}{d^2(x)}\left[\frac{3}{4} + 3z\frac{\partial}{\partial z} + z^2\frac{\partial^2}{\partial z^2}\right]\right\} \mathcal{G}(x, x'; z, z') = \delta(x - x')\delta(z - z'), \tag{3}$$

with flat-boundary conditions, $\mathcal{G}(x, x'; z = 0, z') = \mathcal{G}(x, x'; z = d, z') = 0$. Here the operator $\hat{\mathcal{U}}(x)$ is defined by

$$\hat{\mathcal{U}}(x) = \xi'(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\,\xi'(x) = \xi''(x) + 2\xi'(x)\frac{\partial}{\partial x}. \tag{4}$$

We underline that Eq. (3) is *exact* and valid for any profile $\xi(x)$. It contains a term (in braces) that plays the role of an effective potential. This potential depends not only on the profile $\xi(x)$ (*amplitude scattering*), but also on its first and second derivatives $\xi'(x)$ and $\xi''(x)$ (*gradient scattering*). This very fact demonstrates a highly non-trivial role of surface scattering.

To proceed, we assume that the surface roughness is small in height, $\sigma \ll d$, but can have any value of its slope (σ and R_c can be in arbitrary relation). The small-height approximation is common in surface scattering theories that are based on an appropriate perturbative approach (see for example, Ref. [8]). Using this approach, we obtained the general expression for the inverse attenuation length L_n (or, mean free path) of the n-th conducting subchannel,

$$\frac{1}{L_n} = \frac{1}{L_n^{(1)}} + \frac{1}{L_n^{(2)}}, \tag{5}$$

which is represented as a sum of two terms for a better understanding of the role of amplitude and gradient scattering. The first attenuation length $L_n^{(1)}$ reads as

$$\frac{1}{L_n^{(1)}} = \sigma^2 \frac{(\pi n/d)^2}{k_n d} \sum_{n'=1}^{N_d} \frac{(\pi n'/d)^2}{k_{n'} d} \left[W(k_n + k_{n'}) + W(k_n - k_{n'}) \right], \tag{6}$$

where $k_n = \sqrt{k^2 - (\pi n/d)^2}$, $n = 1, 2, 3, \ldots, N_d$, and N_d is the total number of conducting subchannels. Here the *diagonal term* is formed by the *amplitude mechanism* of surface scattering while the *off-diagonal terms* result from the *gradient scattering*. The above expression exactly coincides with that obtained many years ago by different methods (see, e.g., Ref. [8]). The second attenuation length $L_n^{(2)}$ can be represented in the form,

$$\frac{1}{L_n^{(2)}} = \sum_{n'=1}^{N_d} \frac{1}{L_{nn'}^{(2)}} = \frac{1}{L_{nn}^{(2)}} + \sum_{n' \neq n}^{N_d} \frac{1}{L_{nn'}^{(2)}}, \tag{7}$$

where the diagonal term

$$\frac{1}{L_{nn}^{(2)}} = \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} \left[\frac{1}{3} + \frac{1}{(2\pi n)^2} \right]^2 \left[T(2k_n) + T(0) \right], \tag{8}$$

with $T(k_x) = \int_{-\infty}^{\infty} dx \exp(-ik_x x) \mathcal{W}''^2(x)$ controls the electron/wave scattering *inside* the subchannel (*intramode scattering*). The off-diagonal partial attenuation length $L_{n \neq n'}^{(2)}$ that describes the *intermode scattering* (from n-th subchannel to $n' \neq n$ one), is

$$\frac{1}{L_{nn'}^{(2)}} = \frac{8\sigma^4}{\pi^4} \frac{(\pi n/d)^2}{k_n} \frac{(\pi n'/d)^2}{k_{n'}} \frac{(n^2 + n'^2)^2}{(n^2 - n'^2)^4} \left[T(k_n + k_{n'}) + T(k_n - k_{n'}) \right]. \tag{9}$$

To the best of our knowledge, in the previous studies of a surface scattering the second term in Eq. (5), i.e. $1/L_n^{(2)}$, never was taken into account. In this relation, we should emphasize the principal importance of this term. In spite of that $1/L_n^{(2)}$ is proportional to σ^4, it can prevail over $1/L_n^{(1)}$ even in the small roughness regime $\sigma \ll d$. Indeed, both attenuation lengths, $1/L_n^{(1)}$ and $1/L_n^{(2)}$, depend on R_c via the substantially different functions: the roughness-height power spectrum $W(k_x)$ and the square-gradient power spectrum $T(k_x)$, respectively.

For asymmetric profiles (case (B)) the total width of a waveguide is constant, $d(x) = d$. As a result, the scattering is due to the gradient terms only. Using the above approach one can obtain,

$$L_n^{-1} = \sum_{n'=1}^{N_d} L_{nn'}^{-1}. \tag{10}$$

Remarkably, in this case the diagonal and off-diagonal terms in Eq. (10) are rather distinct. Specifically, the diagonal term is proportional to σ^4,

$$\frac{1}{L_{nn}} = \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} \left[T(2k_n) + T(0)\right], \tag{11}$$

in comparison with off-diagonal terms, which are proportional to σ^2,

$$\frac{1}{L_{nn'}} = 4\sigma^2 \frac{(\pi n/d)^2}{k_n d} \frac{(\pi n'/d)^2}{k_{n'} d} \sin^4 \left[\frac{\pi(n-n')}{2}\right] [W(k_n + k_{n'}) + W(k_n - k_{n'})]. \tag{12}$$

From this equation one can see that due to specific symmetry of the two surface profiles, transitions between subchannels with even difference $n - n'$ are forbidden (corresponding partial scattering lengths diverge). Therefore, only transitions between odd and even subchannels are allowed.

For symmetric profiles (case (C)) the surface scattering is caused by both amplitude and gradient mechanisms. The diagonal term in Eq. (10) has the form,

$$\frac{1}{L_{nn}} = 4\sigma^2 \frac{(\pi n/d)^4}{(k_n d)^2} \left[W(2k_n) + W(0)\right] + \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} \left[\frac{1}{3} + \frac{1}{(\pi n)^2}\right]^2 \left[T(2k_n) + T(0)\right]. \tag{13}$$

According to our analysis, the term which is proportional to σ^2 is due to the amplitude scattering, and the second term ($\propto \sigma^4$) results from the gradient scattering. Note that in a single-mode waveguide with $N_d = 1$ the sum over n' in Eq. (10) contains only one term with $n' = n = 1$. In this case the backscattering length $L_{11}^{(b)}$ which enters into Eqs. (11) and (13) is in accordance with that obtained in Refs. [6, 9].

The off-diagonal partial attenuation length $L_{n \neq n'}$ (intermode scattering) is due to the gradient scattering only,

$$\frac{1}{L_{nn'}} = 4\sigma^2 \frac{(\pi n/d)^2}{k_n d} \frac{(\pi n'/d)^2}{k_{n'} d} \cos^4 \left[\frac{\pi(n-n')}{2}\right] [W(k_n + k_{n'}) + W(k_n - k_{n'})]$$

$$+ \frac{32\sigma^4}{\pi^4} \frac{(\pi n/d)^2}{k_n} \frac{(\pi n'/d)^2}{k_{n'}} \frac{(n^2 + n'^2)^2}{(n^2 - n'^2)^4} \cos^4 \left[\frac{\pi(n-n')}{2}\right] [T(k_n + k_{n'}) + T(k_n - k_{n'})].$$

(14)

The effect of absence of transitions between some subchannels arises in this case, as well as in the case with asymmetric profiles (case (B)). However, in contrast to the former, now there are no transitions between the subchannels with odd difference of their indexes $n - n'$. Thus, only transitions between even subchannels and between odd subchannels are permitted.

In conclusion, we have studied the role of amplitude and gradient scattering in quasi-1D waveguides with rough surfaces. Our results for the models with different symmetries between upper and lower profiles demonstrate a principal difference for these two mechanisms of scattering.

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